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Final Report for AOARD Grant 114017
“Steric Control of Complex Chemical Reactions - I”

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Period of Performance: 14/12/2010 – 13/12/2011

Abstract:

The most exciting result during this period is the one published in *Science* **331**, 900-903 (2011). In that work, we exploited the polarization of an infrared (IR) laser to manipulate the directional property of the reactant, thereby to control the outcomes of a chemical reaction, $\text{Cl} + \text{CHD}_3(v_1=1, \text{IJK} = |10\rangle) \rightarrow \text{HCl}(v=0, 1) + \text{CD}_3(0_0)$. Pronounced impacts are evident not only in total reactivity but also in product state and angular distributions. By contrasting the data with our previously reported stereodynamics in reactions of unpolarized, excited CHD_3 with fluorine [*Science* **325**, 303-306 (2009)] and $\text{O}(^3\text{P})$ [*Chemical Science* **1**, 126-133 (2010)], we elucidated the decisive role of long range anisotropic interactions in steric control of a chemical reaction in general.

Introduction:

The aim of this project is to understand and ultimately to control the reactive outcome of complex systems by vibrational excitations of reactants. Reactions of methane with F, Cl, and $\text{O}(^3\text{P})$ are of prototypical H-atom abstraction mechanism, yet with vastly different energetic and barrier properties. Hence, their contrasting behaviors upon vibrational and translational excitations can serve as benchmark for gaining deeper insights into polyatomic reaction dynamics. Exploiting the product pair-correlation measurement enables us to elucidate the energy flow in the transition-state region of a chemical reaction, and to shed new light onto the mode- and bond-selective chemistry. By pre-aligning the reactant adds an entire new dimension in the field of chemical kinetics and dynamics.

Experiment:

The crossed-beam experiment was performed using the rotating source machine at IAMS, which is equipped with a uniquely designed ion velocity map imaging detector capable of measuring the product pair correlation. The ultrafast femtosecond laser facility is housed in a newly constructed clean room. The installation and tests of the entire laser system is now completed, and some preliminary diagnostic experiments have begun.

Results and Discussion:

The publications listed below described some of the works accomplished. We now extend the investigation of reactant alignment effects on chemical reactivity to the determination of three vector correlation, which is an entirely uncharted territory. The preliminary results are extremely exciting, which opens up the possibility of unfolding the inevitable impact-parameter averaging using the conventional experimental methods.

List of Publications:

SCI publications

1. “Steric Control of the Reaction of CH Stretch-Excited CHD_3 with Chlorine Atom”

- F. Wang, J.-S. Lin, and K. Liu, *Science* **331**, 900-903 (2011).
2. "Imaging the Reaction Dynamics of $O(^3P) + CH_4 \rightarrow OH + CH_3$ "
J. Zhang and K. Liu, *Chemistry - an Asian J.* **6**, 3132-3136 (2011).
 3. "Experimental Signatures for a Resonance-Mediated reaction of Bend-Excited $CD_4(v_b=1)$ with Fluorine Atom"
F. Wang and K. Liu, *J. Phys. Chem. Lett.* **2**, 1421-1425 (2011).
 4. "Quantum Dynamical Resonances in Chemical Reactions: From $A + BC$ to Polyatomic Systems"
K. Liu, *Adv. in Chem. Phys.* **149**, xxx (in press). Invited Review

Invited talks at Conferences (* denoting keynote or plenary lecture)

- *1. "Workshop on Cold and Controlled Collisions", Ringberg Castle, Tegernsee, Germany, Feb. 2-5, 2011.
2. "Cross-Strait Workshop on Chemical Dynamics", Hsinchu, Taiwan, Feb. 18-21, 2011.
- *3. "Marie Curie ICONIC Training School", Paris, France, June 6-11, 2011.
- *4. "XXIII Conference on Dynamics of Molecular Collisions-DMC", Snowbird, Salt Lake City, UT, USA, July 10-15, 2011.
- *5. "The 31st International Symposium on Free Radicals", Port Douglas, Australia, July 24-29, 2011.
- *6. "Conference on Molecular Energy Transfer - COMET", Jesus College, Oxford, UK, Sept. 11-16, 2011.
7. "Sustainable Energy Workshop", IAMS, Taipei, Taiwan, Dec. 15-16, 2011.